Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

First-principles investigation of band offsets and dielectric properties of Silicon-Silicon Nitride interfaces[1] TUAN ANH PHAM, Department of Chemistry, UC Davis, TIANSHU LI, Department of Chemistry, UC Davis and Department of Civil and Enviromental Engineering, The George Washington University, FRANCOIS GYGI, Department of Applied Science and Department of Computer Science, UC Davis, GIULIA GALLI, Department of Chemistry and Department of Physics, UC Davis — Silicon Nitride (Si3N4) is a possible candidate material to replace or be alloyed with SiO2 to form high-K dielectric films on Si substrates, so as to help prevent leakage currents in modern CMOS transistors. Building on our previous work on dielectric properties of crystalline and amorphous Si3N4 slabs [1], we present an analysis of the band offsets and dielectric properties of crystalline-Si/amorphous Si3N4 interfaces based on first principles calculations. We discuss shortcomings of the conventional bulk-plus line up approach in band offset calculations for systems with an amorphous component, and we present the results of band offsets obtained from calculations of local density of states. Finally, we describe the role of bonding configurations in determining band edges and dielectric constants at the interface.

[1] T. Anh Pham et al., Appl. Phys. Lett., 96, 062902 (2010).

[1]We acknowledge financial support from Intel Corporation.

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Date submitted: 08 Dec 2010 Electronic form version 1.4